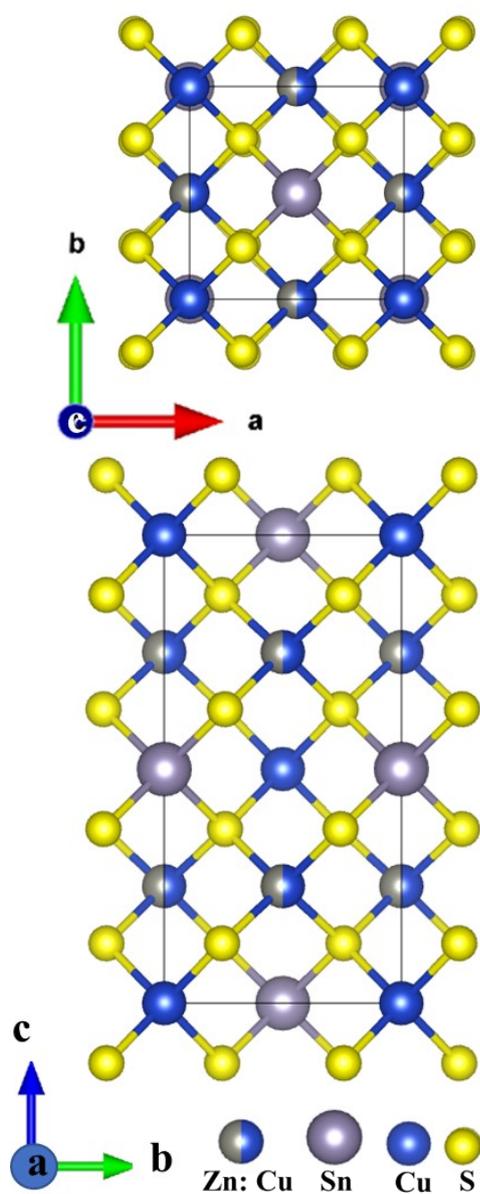


ARTICLE

Dual-Functionality of CZTS Nanoflakes: Anode material for Lithium-ion batteries and as counter electrodes in DSSCs - A DFT and Experimental Investigation

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G. Rajesh^{*(a)(b)}, M.R. Venkatraman^(d), Ramesh Sivasamy^(e), Sreejith P Madhusudan^(f), Helen Annal Therese^(c), Jeyakiruba Palraj^{†(c)}, Marcos Flores^(b)

DSSC fabrication:

The commercial TiO₂ paste was procured and diluted slightly by the addition of a few drops of ethanol, and it was mixed thoroughly to obtain a homogeneous paste. The as-prepared paste was coated over 40 mM TiCl₄ pre-treated FTO substrates (Fluorine doped Tin Oxide) by doctor blade method. The thickness of the coated layer was about 10 μm. The prepared photoanodes were further subjected to heat treatment at 450 °C for 1 hour in a muffle furnace. The prepared films were also post-treated with 40 mM TiCl₄ at 70 °C for 20 min and it is annealed at 450 °C for 30 min. The sensitization of the prepared

electrodes was carried out by soaking in ethanolic 0.3 mM N719 dye solution at room temperature for 12 hours in a dark environment. After sensitization, the dye-soaked electrodes were taken out and washed with anhydrous alcohol for the complete removal of the excess un-anchored dye molecules. For the construction of DSSC, the prepared CZTS and Pt-coated FTOs were used as counter electrodes and Iodine redox (Iodolyte HI-30, Solaronix) was used as electrolyte. Dye-sensitized solar cells were constructed with the structure FTO/TiO₂-Dye/redox electrolyte/CZTS/Pt-FTO and the active area of the cell was 0.25 cm².

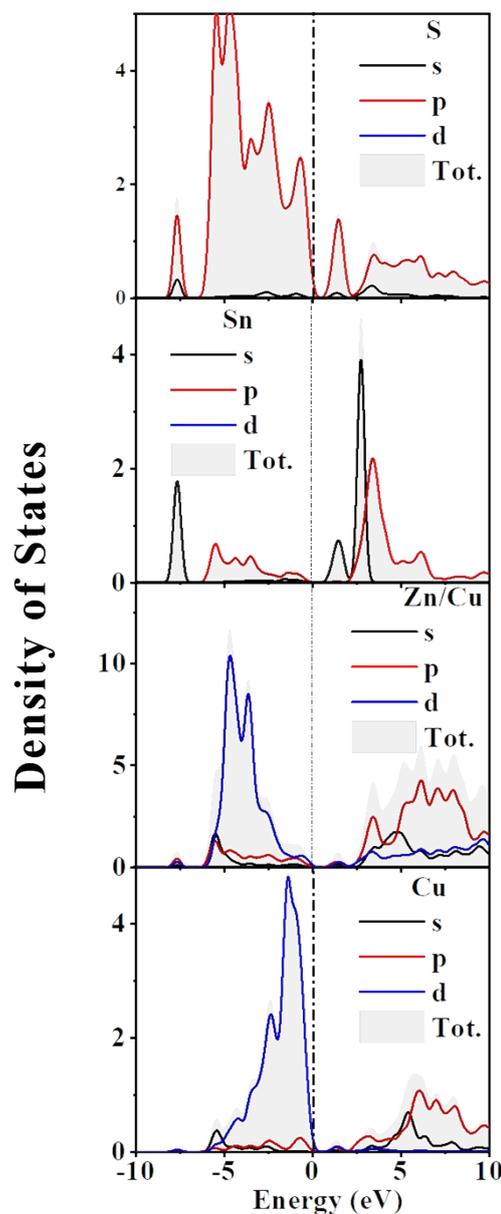
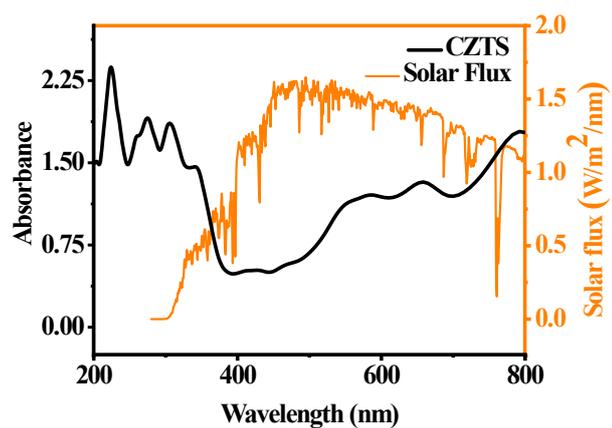


Figure S2. The site-projected density of states of the CZTS nanoparticles

Table S1 Refined CZTS Crystal structure data

Elements	x	y	z	Occ	Wyckoff position
Cu	0.00000	0.50000	0.25000	0.500	4d
Zn	0.00000	0.50000	0.25000	0.500	4d
Cu	0.00000	0.00000	0.00000	1.000	2a
Sn	0.00000	0.00000	0.50000	1.000	2b
S	0.24383	0.24383	0.12792	1.000	8i

**Figure S3** Optical absorption spectra of CZTS material compared with the standard solar spectrum